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Simulating Ion Irradiation of Surfaces: A comparison of Binary Collision Approximation and Molecular Dynamics Models to Laboratory Measurements

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ABSTRACT

Surface sputtering by solar-wind ion irradiation of airless planetary bodies is important for understanding the body's surface and exospheric compositions. Laboratory simulations are both complex and expensive, and obtaining field data is even more challenging. Hence, theoretical sputtering models are used to describe the behavior of the incoming ions, impacted surface, and sputtered atoms. These results can then be used as inputs for exospheric models. The most common sputter models use the binary collision approximation (BCA), such as SDTrimSP. While these models are typically accurate for high impact energies, the approximations can potentially introduce error for low energy impacts or crystalline targets. In contrast, Molecular Dynamics (MD) simulations remove the BCA approximation and are able to simulate the entire collision cascade, albeit at a high computational cost. MD simulations also allow one to control the properties of the initial substrate, including crystalline structure, temperature, crystal damage, and roughness. However, MD simulations can require several user specific choices, such as interatomic potential, that can affect accuracy. Therefore, before these models can be confidently used to simulate planetary surface ion impacts, it is important to verify their ranges of applicability and limitations by comparison to pre-existing experimental values. In specific, we consider a copper substrate impacted by argon ions with kinetic energies between 200-1000 eV and compare the MD and SDTrimSP results to the experimental sputtering yield and energy distributions. Our results indicate that for higher energy impacts, both BCA and MD methods can be used to accurately predict the yield and energy distribution of sputtered atoms. However, as impact energies are decreased, extended collision cascades can no longer develop in the impacted substrate. As a result, anisotropic effects are increased, and energy distributions can no longer confidently be predicted via the commonly used BCA Thompson distribution. Results from both SDTrimSP and MD had better agreement with experimental data and closely agreed with each other. Further, experimental results often measure only normal emissions and are therefore likely subject to a narrowing of energy distributions caused by emission angle anisotropies. In contrast, our simulation results account for the entire distribution of emission angles and therefore eliminate this potentially overlooked anisotropic effect.

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